Data driven peak and reachability set estimation

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Main Ideas

L_∞ bounded noise setting yields polytopic constraints

Use polytopic structure to simplify nonpositivity

Apply to Peak and Reachable Set Estimation

Peak Estimation Background

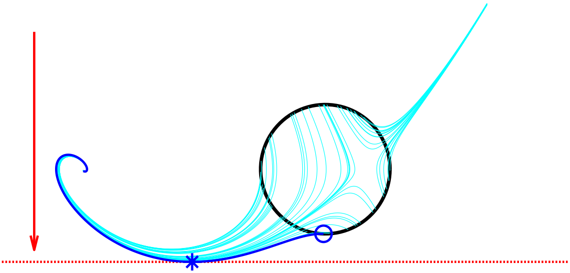
Peak Estimation Problem

Find maximum value of $p(x)$ along trajectories

$$P^* = \max_{t,\ x_0 \in X_0} p(x(t))$$

$$\dot{x}(t) = f(t, x(t)) \qquad\qquad t \in [0, T]$$

$$x(0) = x_0 \in X_0$$



$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3]$$

Peak Function Program

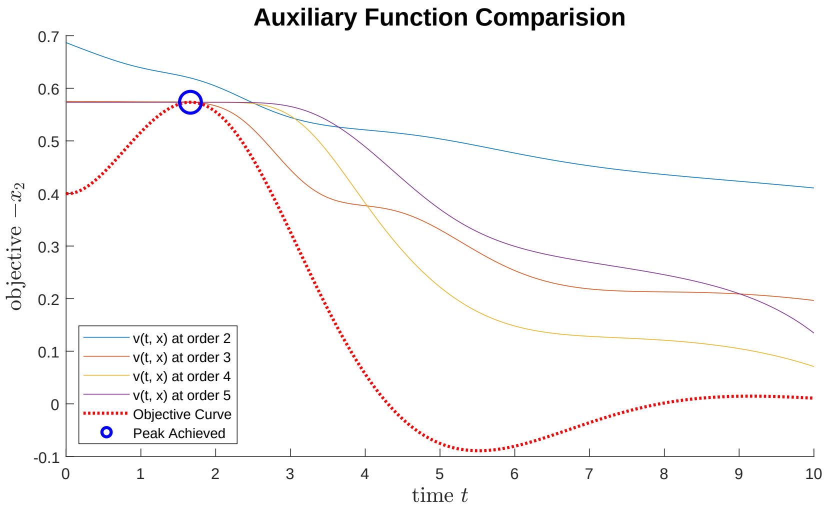
Infinite dimensional linear program (Fantuzzi, Goluskin, 2020)

Uses auxiliary function $v(t, x)$

$$
\begin{aligned}
d^* = \min_{\gamma \in \mathbb{R}} \quad & \gamma \\
& \gamma \geq v(0, x) && \forall x \in X_0 \\
& \mathcal{L}_f v(t, x) \leq 0 && \forall (t, x) \in [0, T] \times X \\
& v(t, x) \geq p(x) && \forall (t, x) \in [0, T] \times X \\
& v \in C^1([0, T] \times X)
\end{aligned}
$$

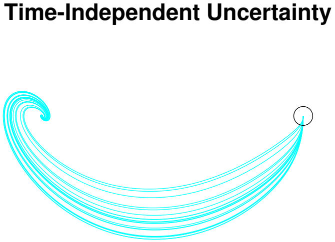
$P^* = d^*$ holds if $[0, T] \times X$ is compact, f Lipschitz

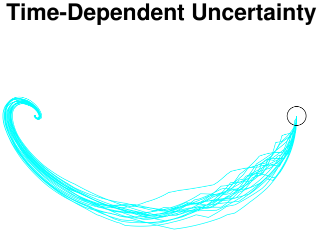
Auxiliary Evaluation along Optimal Trajectory



Optimal $v(t, x)$ should be constant until peak is achieved

System with Uncertainty Example





$$\dot{x} = [x_2, -x_1 w - x_2 + x_1^3/3]$$

$$w \in [0.5, 1.5],\ \ x_0 = [1; 0]$$

Peak Estimation with Uncertainty

Dynamics $\dot{x} = f(t, x(t), w(t))$

Uncertain process $w(t) \in W, \ \forall t \in [0, T]$

Time-dependent w

$$\mathcal{L}_f v(t, x) \leq 0 \qquad \forall (t, x, w) \in \forall [0, T] \times X \times W$$

Time-independent w ($\frac{dw}{dt} = 0$)

$$\mathcal{L}_f v(t, x, w) \leq 0 \qquad \forall (t, x, w) \in [0, T] \times X \times W$$

Data Driven Setting

Noise Model

Ground truth $\dot{x} = F(t, x)$

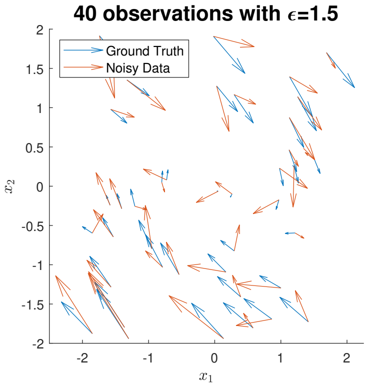
Corrupted observations of system F in $t \in [0, T]$

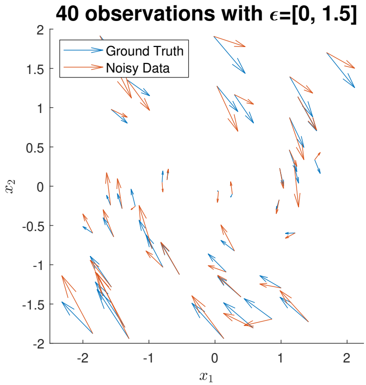
$$(t_j, x_j, \dot{x}_j) \qquad \forall j = 1, \ldots, N_s$$

Assumption of L_∞ bounded noise

$$\|F(t_j, x_j) - \dot{x}_j\|_\infty \leq \epsilon \qquad \forall j = 1, \ldots, N_s$$

Sampling: Flow System





$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3]$$

Dynamics Model

Parameterize unknown F by functions in dictionary

$$\dot{x}(t) = f(t, x, w) = f_0(t, x) + \sum_{\ell=1}^{L} w_\ell f_\ell(t, x)$$

Affine in uncertainties w

Bounded noise constraint ϵ

$$\begin{aligned} \|F(t_j, x_j) - \dot{x}_j\|_\infty &\leq \epsilon & \qquad \forall j = 1, \ldots, N_s \\ \|f(t_j, x_j, w) - \dot{x}_j\|_\infty &\leq \epsilon & \qquad \forall j = 1, \ldots, N_s \end{aligned}$$

Noise Constraints

2 linear constraints for each coordinate i, sample j

$$-\epsilon \leq f_0(t_j, x_j)_i + \sum_{\ell=1}^{L} w_\ell f_\ell(t_j, x_j)_i - (\dot{x}_j)_i \leq \epsilon$$

Polytopic region $W = \{w \in \mathbb{R}^L \mid Aw \leq b\}$ with $b \in \mathbb{R}^{2N_x N_s}$

Prior Work

Data Driven Solving Methods:

- Interval Analysis
- Koopman Operators
- Infinite LPs
- SVM/Deep Learning

Data Driven Polytopic Framework:

- Safety Verification
- Stabilizing and Safe Control (barrier/density)

Summary of Assumptions

Set $[0, T] \times X$ is compact

Dynamics $f(t, x, w)$ are Lipschitz, affine in w

Uncertainty W is a compact polytope $\{w \mid Aw \leq b\}$

Nonempty interior: $\exists w \in \mathbb{R}^L \mid Aw < b$

Constraint Decomposition

Feasibility Pair

Setting of time-dependent uncertainty $w(t) \in W$

Problem is Feasible

$$\mathcal{L}_{f(t,x,w)} v(t,x) \leq 0 \qquad \forall (t,x,w) \in [0,T] \times X \times W$$

Problem is Infeasible

$$\mathcal{L}_{f(t,x,w)} v(t,x) > 0 \qquad \exists (t,x,w) \in [0,T] \times X \times W$$

Pair of Strong Alternatives

Inequalities and Multipliers

One strict inequality, m non-strict inequalities

$$R = \{w \mid H(w) > 0, h_1(w) \geq 0, \ldots, h_m(w) \geq 0\}$$

Define weighted sum with multipliers $\zeta \geq 0$

$$S(w;\zeta) = H(w) + \sum_{k=1}^{m} \zeta_k h_k(w)$$

S is positive for all $w \in R,\ \zeta \geq 0$

Theorem of Alternatives

Lagrange dual function g

$$g(\zeta) = \sup_{w \in \mathbb{R}^L} S(w; \zeta) = \sup_{w \in \mathbb{R}^L} H(w) + \sum_{k=1}^{m} \zeta_k h_k(w)$$

Certificate ζ that R is empty:

$$g(\zeta) \leq 0 \qquad \forall \zeta \geq 0$$

Weak alternative $g(\zeta) \leq 0$ is strong if:

- $H(w)$, $\forall_k h_k(w)$ convex in w
- Exists a point $w : \forall_k h_k(w) > 0$ (Slater)

Apply Alternatives

Region $R = \{w \mid \mathcal{L}_f v(t,x) > 0,\ Aw \leq b\}$

Form Lagrange dual $g(\zeta; v) = \sup_{w \in \mathbb{R}^L} S(w; \zeta, t, x)$:

$$g(\zeta; v) = \begin{cases} \mathcal{L}_{f_0} v + b^T \zeta & (A^T)_\ell \zeta - f_\ell \cdot \nabla_x v = 0 \quad \forall \ell \\ \infty & \text{else} \end{cases}$$

Bounded g requires equality constraints over $[0, T] \times X$

Lie Polytopic Decomposition

Original

$$\mathcal{L}_f v(t,x) \leq 0 \qquad \forall (t,x,w) \in [0,T] \times X \times W$$

Decomposed

$$\begin{aligned}
&\mathcal{L}_{f_0} v(t,x) + b^T \zeta(t,x) \leq 0 && \forall (t,x) \in [0,T] \times X \\
&(A^T)_\ell \zeta(t,x) = f_\ell \cdot \nabla_x v(t,x) && \forall \ell = 1, \ldots, L \\
&\zeta_k(t,x) \in C_+([0,T] \times X) && \forall k = 1, \ldots, m
\end{aligned}$$

Strong equivalence (given convexity in w)

Summary of Relaxations

Time-independent to time-dependent uncertainty

Nonnegativity to Sum of Squares

Sum of Squares at finite degree

Peak Estimation (revisited)

Peak Original Program

Include time-varying uncertainty $w(t) \in W$

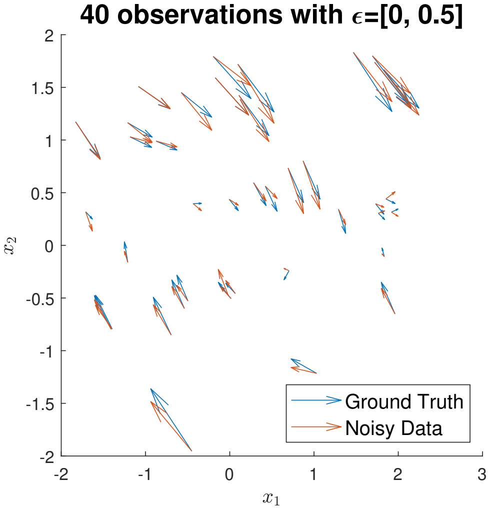
$$
\begin{aligned}
d^* = \min_{\gamma \in \mathbb{R}} \quad & \gamma \\
& \gamma \geq v(0, x) && \forall x \in X_0 \\
& \mathcal{L}_f v(t, x) \leq 0 && \forall (t, x, w) \in [0, T] \times X \times W \\
& v(t, x) \geq p(x) && \forall (t, x) \in [0, T] \times X \\
& v \in C^1([0, T] \times X)
\end{aligned}
$$

Peak Decomposed Program

Only the Lie Derivative constraint changes

$$
\begin{aligned}
d^* = \; & \min_{\gamma \in \mathbb{R}} \gamma \\
& \gamma \geq v(0, x) && \forall x \in X_0 \\
& \mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 && \forall (t, x) \in [0, T] \times X \\
& (A^T)_\ell \zeta(t, x) = (f_\ell \cdot \nabla_x) v(t, x) && \forall \ell = 1, \ldots, L \\
& v(t, x) \geq p(x) && \forall (t, x) \in [0, T] \times X \\
& v(t, x) \in C^1([0, T] \times X) \\
& \zeta_k(t) \in C_+([0, T] \times X) && \forall k = 1, \ldots, m
\end{aligned}
$$

Peak Estimation Example (Flow)



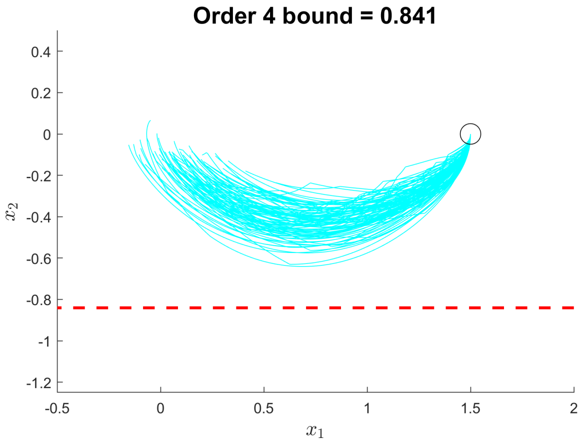
$$\dot{x} = [x_2,\ -x_1 - x_2 + x_1^3/3],\ \ T = 5$$

Peak Estimation Example (Flow)

$$\dot{x} = [x_2,\ -wx_1 - x_2 + x_1^3/3]$$

$$L = 1,\ m = 80 \text{ (2 nonredundant)}$$

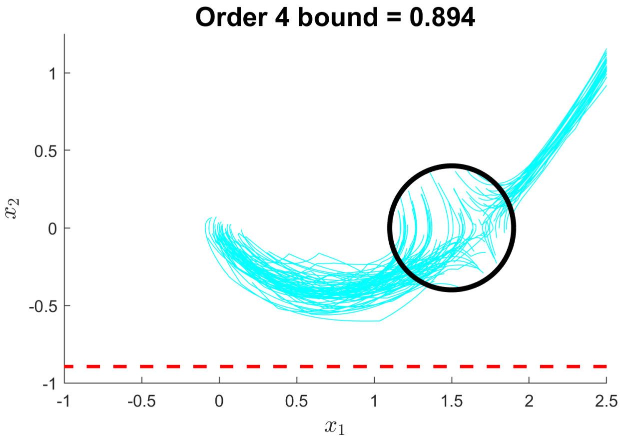
Peak Estimation Example (Flow)



$$\dot{x} = [x_2,\ \text{cubic}(x_1, x_2)]$$

$$L = 10,\ \ m = 80\ (33 \text{ nonredundant})$$

Peak Estimation Example (Flow)



$$\dot{x} = [x_2,\ \text{cubic}(x_1, x_2)]$$

$$X_0 = \{x \mid (x_1 - 1.5)^2 + x_2 \leq 0.4^2\}$$

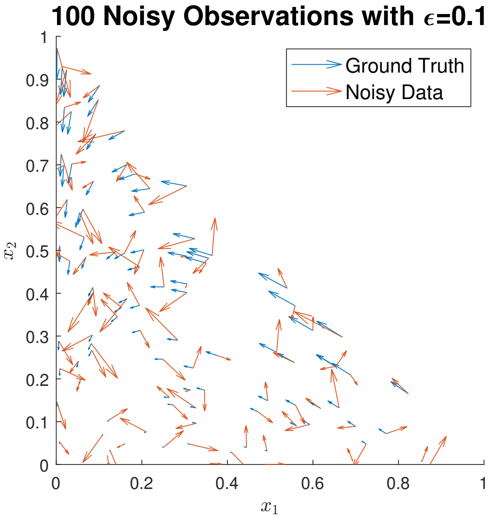
Peak Estimation Example (Epidemic)

Dynamics model:

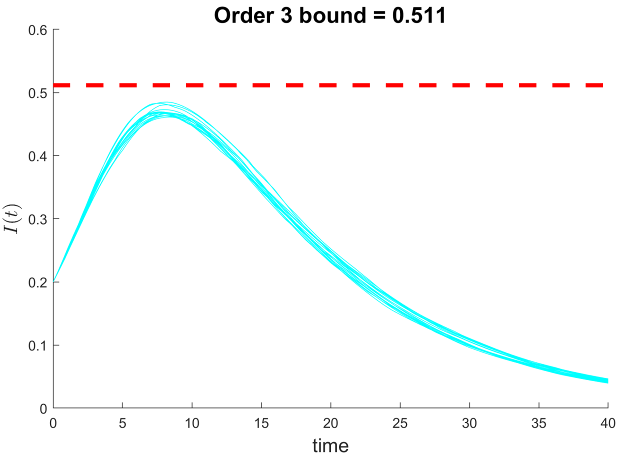
$$S' = -\beta S I$$
$$I' = \beta S I - \gamma I$$

Truth: $\beta = 0.4, \ \gamma = 0.1$

$m = 400$ constraints



Peak Estimation Example (Epidemic)



$T = 40$, Unknown (β, γ)

$L = 2$, $m = 400$ (5 nonredundant)

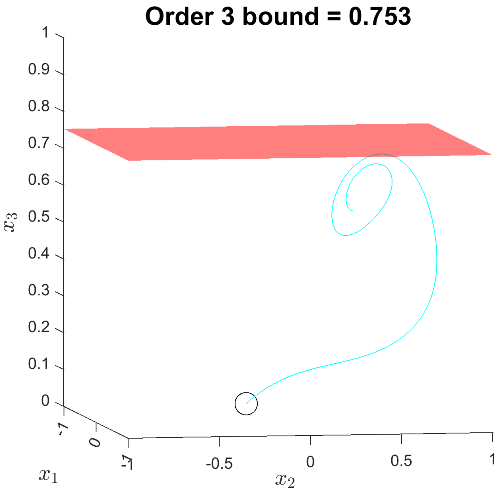
Peak Estimation Example (Twist)

Dynamics model:

$$\dot{x}_i = A_{ij}x_j - B_{ij}(4x_j^3 - 3x_j)$$

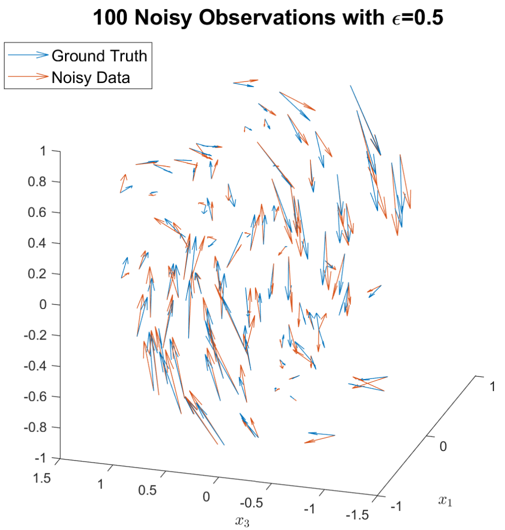
$$A = \begin{bmatrix} -1 & 1 & 1 \\ -1 & 0 & -1 \\ 0 & 1 & -2 \end{bmatrix}$$

$$B = \begin{bmatrix} -\frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$



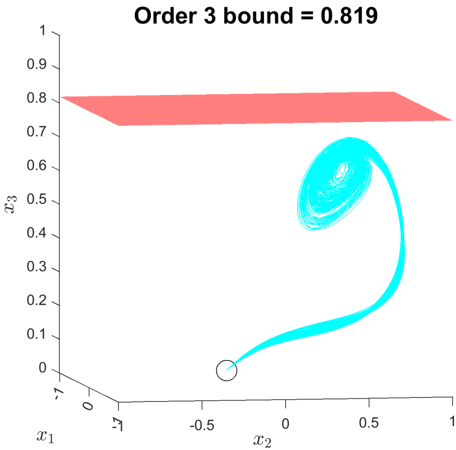
$$X_0 = [-1, 0, 0], \quad T = 8$$

Peak Estimation Example (Twist)



$$m = 2N_sN_x = 600 \text{ constraints}$$

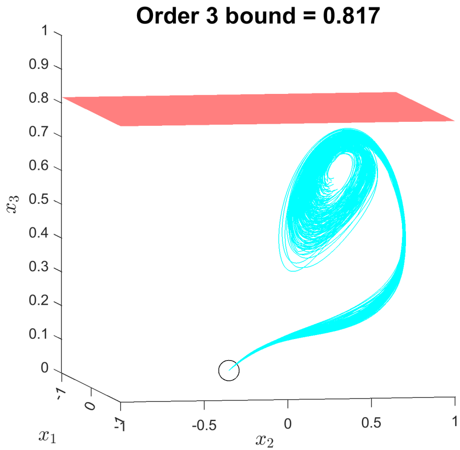
Peak Estimation Example (Twist)



Unknown A, Known B

$L = 9, \;\; m = 600$ (34 nonredundant)

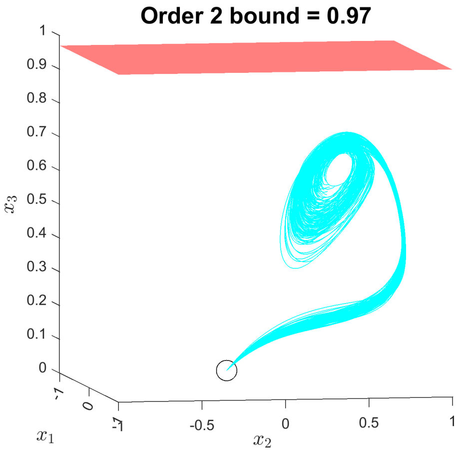
Peak Estimation Example (Twist)



Known A, Unknown B

$$L = 9, \;\; m = 600 \text{ (30 nonredundant)}$$

Peak Estimation Example (Twist)



Unknown A, Unknown B

$L = 18, \;\; m = 600$ (70 nonredundant)

Reachable Set Estimation

Reachable Set Estimation

Find set of states reachable from $x_0 \in X_0$ at time $t = T$

$$
\begin{aligned}
P^* = \max_{X_T \subseteq X} \ & \mathrm{vol}(X_T) \\
& X_T : \ \exists x(t \mid x_h) : \\
& \qquad \dot{x}(t) = f(t, x(t), w(t)) && \forall t \in [0, T] \\
& \qquad w(t) \in W && \forall t \in [0, T] \\
& \qquad x(0) \in X_0, \ x(T) \in X_T
\end{aligned}
$$

Indicator Function Approximation

Reachability indicator function χ_T

$$\chi_T(x) = \begin{cases} 1 & x \in X_T \\ 0 & x \notin X_T \end{cases}$$

Create upper bound approximant $\omega(x) \in C(X)$:

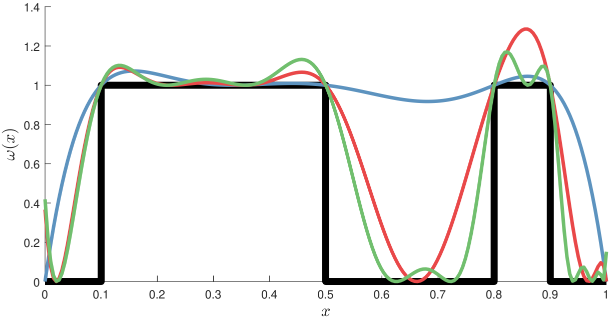
$$\begin{aligned} \omega(x) &\geq 1 && \forall x \in X_T \subseteq X \\ \omega(x) &\geq 0 && \forall x \in X \end{aligned}$$

Stone-Weierstrass: $\omega(x)$ is polynomial

Indicator Function Approximation Example

Determine quality by comparing $\int_X \omega(x)dx$ vs $\mathrm{vol}(X_T)$

$$X_T = [0.1, 0.5] \cup [0.8, 0.9]$$



Function	$d = 6$	$d = 20$	$d = 120$	Truth
Area	0.927	0.734	0.671	0.5

Reachable Set Standard Program

Infinite dimensional linear program (Henrion, Korda, 2012)

$$
\begin{aligned}
d^* = \ \min \int_X \omega(x)dx \\
& v(0,x) \le 0 && \forall x \in X_0 \\
& \mathcal{L}_{f(t,x,w)} v(t,x) \le 0 && \forall (t,x,w) \in [0,T] \times X \times W \\
& v(T,x) + \omega(x) \ge 1 && \forall x \in X \\
& v(t,x) \in C^1([0,T] \times X) \\
& \omega(x) \in C_+(X)
\end{aligned}
$$

Approximation $X_T \subset \{x \in X \mid \omega(x) \ge 1\}$

Reachable Set Decomposed Program

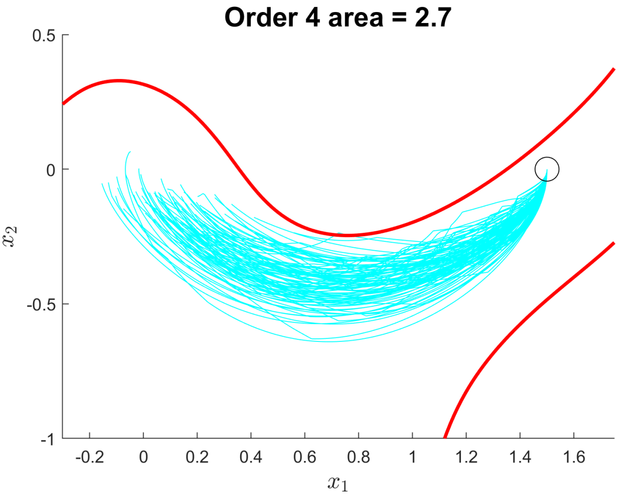
Approximation $X_T \subset \{x \in X \mid \omega(x) \geq 1\}$

$$
\begin{aligned}
d^* = \ \min \int_X \omega(x)dx & \\
v(0, x) \leq 0 & \quad \forall x \in X_0 \\
\mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 & \quad \forall (t, x) \in [0, T] \times X \\
(A^T)_\ell \zeta(t, x) = (f_\ell \cdot \nabla_x) v(t, x) & \quad \forall \ell = 1, \ldots, L \\
v(T, x) + \omega(x) \geq 1 & \quad \forall x \in X \\
v(t, x) \in C^1([0, T] \times X) & \\
\omega(x) \in C_+(X) & \\
\zeta_k(t) \in C_+([0, T] \times X) & \quad \forall k = 1, \ldots, m
\end{aligned}
$$

Reachable Set Estimation Example (Flow)

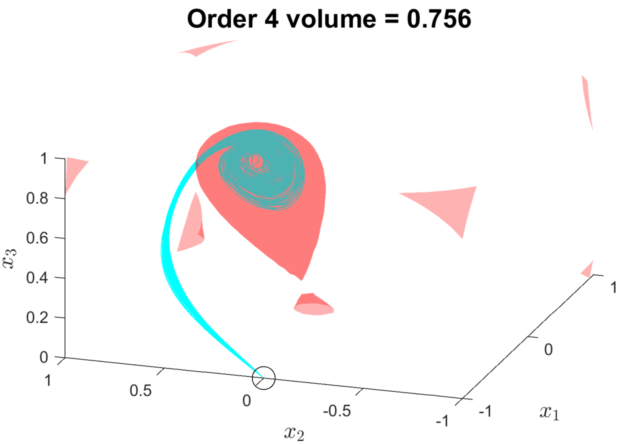
$L = 1, \; m = 80$ (2 nonredundant)

Reachable Set Estimation Example (Flow)



$L = 10, \;\; m = 80$ (33 nonredundant)

Reachable Set Estimation Example (Flow)



Unknown A, Known B

$L = 9, \; m = 600$ (34 nonredundant)

Take-aways

Conclusion

Exploit polytopic structure of L_∞-bounded noise

More SOS constraints in fewer variables

Tractable optimization problems (after preprocessing)

Future Work

- Streaming data and warm starts
- Time-space partitioning
- Maximum positively invariant sets
- Optimal control and extraction
- Hybrid systems
- Compatibility with structure (e.g. sparsity)

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National Science Foundation

Air Force Office of Scientific Research

Thank you

Thank you for your attention

Extra Material

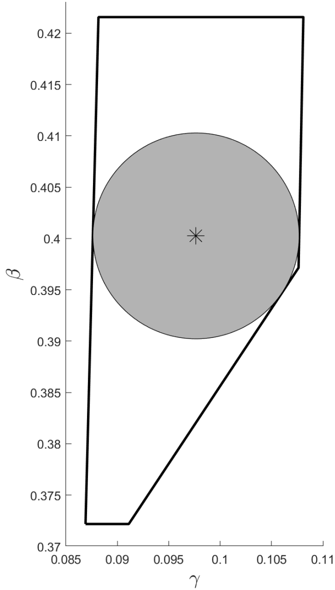
Preprocessing: Centering

Chebyshev center c: center of sphere with largest radius in W

Find through linear programming

$$
\begin{aligned}
&\max r \\
&A_k c + r\|A_k\|_2 \leq b_k \qquad \forall k \\
&r \geq 0, c \in \mathbb{R}^L
\end{aligned}
$$

Shifted dynamics $f_0 \leftarrow f_0 + \sum_{\ell=1}^{L} c_\ell f_\ell$

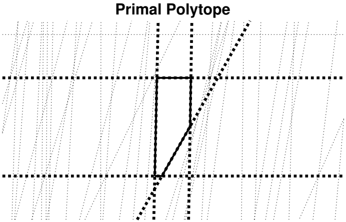


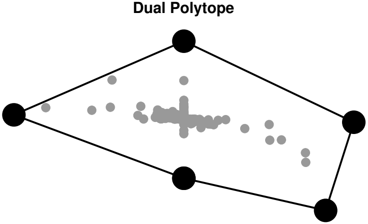
Preprocessing: Redundancy

Majority of $m = 2N_xN_s$ constraints are often redundant

Convex hull of dual polytope:
Time: $\Omega(m \log m + m^{\lfloor L/2 \rfloor})$

Linear program per constraint:
Time: $m \times \tilde{O}(mL + L^3)$
(Jan van den Brand *et. al.* 2020)





Variations: Nonnegative Control

Control set is $W = \{w \mid Aw \leq b,\ w \geq 0\}$

$$\begin{aligned}
&\mathcal{L}_{f_0} v(t,x) + b^T \zeta(t,x) \leq 0 && \forall (t,x) \in [0,T] \times X \\
&(A^T)_\ell \zeta(t,x) \geq f_\ell \cdot \nabla_x v(t,x) && \forall (t,x) \in [0,T] \times X, \forall \ell \\
&\zeta_k(t,x) \in C_+([0,T] \times X) && \forall k = 1, \ldots, m
\end{aligned}$$

Mix $\geq$ and $=$ depending on input structure

Variations: Centrally Symmetric Control Set

If $w \in W$, then $-w \in W$

Control set is $W = \{w \mid -b \leq Aw \leq b\}$

$$\begin{aligned}
&\mathcal{L}_{f_0} v(t,x) + b^T \zeta(t,x) \leq 0 && \forall (t,x) \in [0,T] \times X \\
&(A^T)_\ell \zeta(t,x) \geq |f_\ell \cdot \nabla_x v(t,x)| && \forall (t,x) \in [0,T] \times X, \forall \ell \\
&\zeta_k(t,x) \in C_+([0,T] \times X) && \forall k = 1, \ldots, m
\end{aligned}$$

Generalization of "Convex Optimization of Nonlinear Feedback Controllers via Occupation Measures" by Majumdar *et. al.* $(A = I, b = 1)$